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# Simulation of the effects of interstitial content and temperature on texture and substructure evolution of commercially pure titanium during ECAP

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**Abstract.** The effects of interstitial content and temperature on texture and substructure evolution of commercially pure titanium during the first pass of equal channel angular pressing were investigated. Different values of critical resolved shear stresses were proposed for different interstitial contents and processing temperatures. Simulation results show that texture was affected by both interstitial element and temperature. Also, in substructure simulation, the cell size was affected by interstitial content, while the fragment size was more dependent on temperature change.

## 1. Introduction

Commercially pure (CP) titanium with hexagonal crystal structure develops strong textures during deformation due to the uneven activation of dislocation glide and twinning systems, in which five modes are generally considered, i.e. prismatic  $\langle a \rangle$  slip, basal  $\langle a \rangle$  slip, first order pyramidal  $\langle c + a \rangle$  slip,  $\{10\bar{1}2\}\langle 10\bar{1}\bar{1} \rangle$  tensile twin, and  $\{11\bar{2}2\}\langle \bar{1}\bar{1}23 \rangle$  compressive twin. The activation of different modes in deformation, and thus the texture and substructure evolution are quite sensitive to the detailed material and process parameters. Therefore, the present paper is discussing the response of the modelling framework proposed by Seefeldt and Guo in this volume to variations of the interstitial content and the processing temperature.

## 2. Simulation details

### 2.1. Simulation setup

Two temperatures, 298K and 473K, and two interstitial contents, Grade 1 and Grade 4 with an oxygen equivalent content of 1800 ppm and 4000 ppm respectively, were studied. The virtual die of ECAP had an intersection angle of  $\Phi = 90^\circ$ . The imposed strain for one pass was 1.15 and the strain rate was  $10^{-3}/s$ . The initial texture was random. More details involved in simulation were referred to the model description in this volume.

### 2.2. Effect of interstitial content and temperature on simulation parameters

In the texture simulation, the interstitial content and the temperature enter only through  $\tau_c$ . Several experimental and simulation works have used different selections of  $\tau_c$  [1–6]. Besides, Conrad [4] also reported that,  $\tau_c$  of dislocation slip increase with increasing interstitial content



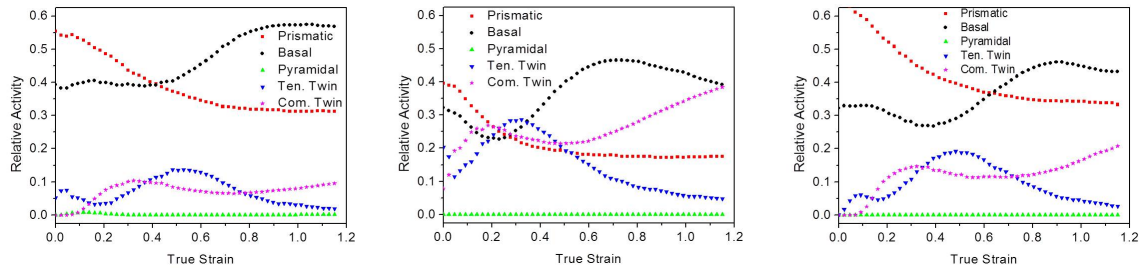
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**Table 1.**  $\tau_c$  (in MPa) of slip and twinning modes used with respect to interstitial element content and temperature [4–6].

Interstitial Content	Temperature	Prismatic	Basal	Pyramidal	Tens. Twin	Comp. Twin
Grade 1	298K	75	100	250	150	300
Grade 4	298K	120	150	300	120	200
Grade 4	473K	35	60	200	120	200

or decreasing temperature, while for twinning, it has a different tendency that  $\tau_c$  of twin systems increase with decreasing interstitial element content and keep unchanged with changing temperature. Based on these studies, in this paper,  $\tau_c$  of slip and twinning modes were deduced for two interstitial contents and two temperatures, see table 1.

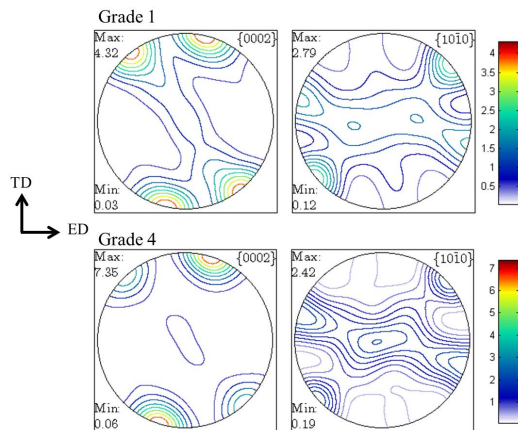
The interstitial content will also change the stacking fault energy (SFE) significantly [6], and thus cross-slip, dislocation annihilation and multiplication. However, by lack of experimental or theoretical estimations for this dependency, SFE data calculated in high purity titanium are used [7], and the effect of interstitial content on SFE was neglected.

**Figure 1.** Slip activities of slip and twinning modes during the first pass for materials (left) Grade 1 at 298K; (mid) Grade 4 at 298K; (right) Grade 4 at 473K .

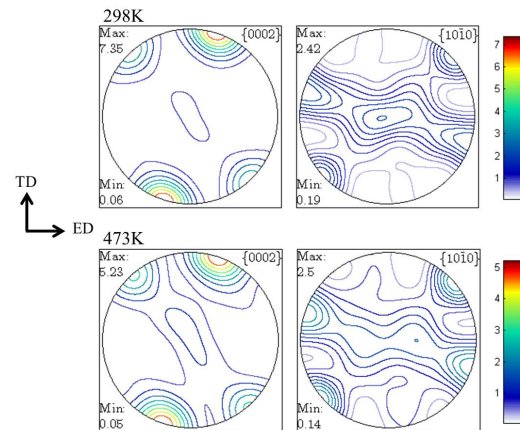
### 3. Results and discussion

#### 3.1. Texture evolution

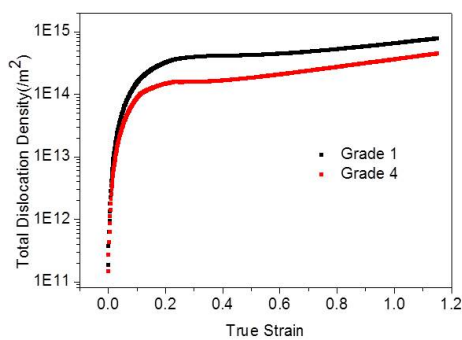
Figure 1 shows the slip activities of all deformation modes for three simulations with different interstitial contents and process temperatures. Figure 2 and 3 present the texture evolution during the first pass with interstitial content change and temperature change, respectively. By comparing the left and middle images in Figure 1, prismatic  $\langle a \rangle$  and basal  $\langle a \rangle$  slip are suppressed with increasing of interstitial content, while two twin modes are promoted, thus the texture component along the normal shear direction which is mainly attributed to prismatic  $\langle a \rangle$  and basal  $\langle a \rangle$  slip becomes weaker with higher interstitial content. Moreover, by comparing the middle and right images in Figure 1, we can see that, at 473K, the prismatic  $\langle a \rangle$  slip is promoted and twins are suppressed. Basal  $\langle a \rangle$  slip keeps almost unchanged. Therefore, as shown in Figure 3, higher temperature strengthens the texture component at normal shear direction. For all simulations, the pyramidal  $\langle c + a \rangle$  slip has a negligible contribution to the deformation. The results are in line with previous findings and match well with experimental observations, e.g. by Saiyi Li's work [8].



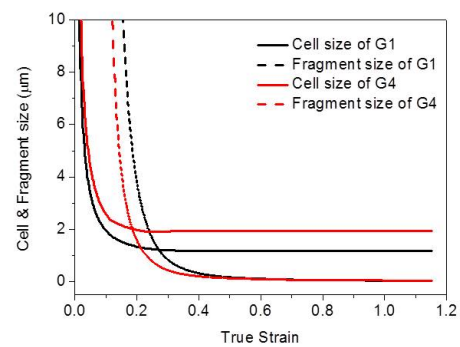
**Figure 2.** Simulated texture after one pass for Grade 1 and Grade 4 at 298K.



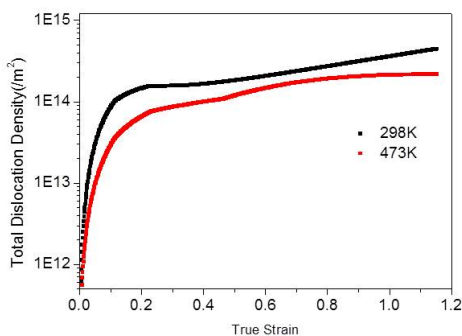
**Figure 3.** Simulated texture after one pass at 298K and 473K.



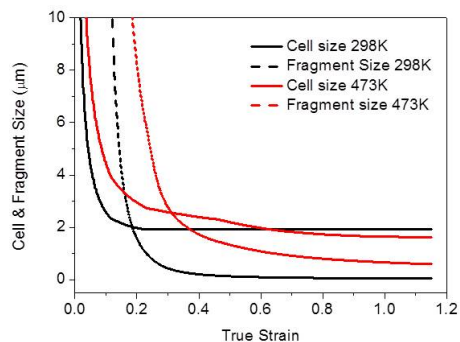
**Figure 4.** Total dislocation density of Grade 1 and Grade 4 CP titanium at 298K.



**Figure 5.** Cell and fragment size of Grade 1 and Grade 4 CP titanium at 298K.



**Figure 6.** Total dislocation density of a Grade 4 CP titanium at 298K and 473K.



**Figure 7.** Cell and fragment size of a Grade 4 CP titanium at 298K and 473K.

### 3.2. Substructure evolution

The effects of interstitial content and temperature on substructure evolution are discussed in terms of total dislocation densities and cell and fragment size evolution. The cell and fragment

sizes are calculated via scaling laws from the total dislocation density and from the fragment boundary surface density. Figure 4 shows that, the total dislocation density was decreased with increasing interstitial content, indicating that the suppressed activities of dislocation slip with more interstitial content resulted in a decrease of total dislocation density. Therefore, as shown in Figure 5, the saturation value of cell size increased from about  $1.2\ \mu\text{m}$  in Grade 1 to about  $2\ \mu\text{m}$  in Grade 4 materials. The saturation value of fragment size were almost unchanged. On the effect of temperature, in Figure 6, a decreasing trend of total dislocation density was observed with increasing temperature. The cell size was almost the same, however, the saturation value of fragment size was higher at an elevated temperature. This simulation result indicates that interstitial element affects the evolution of cell structure while temperature affects the evolution of fragment structure. Experimental observations on substructure evolution of pure titanium during ECAP are referred to the works of Kim et al. [9], Gunderov et al. [10], Zhao et al. [11, 12]

#### 4. Conclusion

The effects of interstitial content and temperature on texture and substructure evolution of CP titanium materials were investigated for the first pass of ECAP. Simulation results show that prismatic and basal slip were suppressed and twinning was promoted at lower temperature or with higher interstitial content. Also, the saturation value of cell size was mostly affected by interstitial element content, while the fragment size was more dependent on the temperature change.

#### Acknowledgment

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